



chain nodes :

15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38
 39 46 47 48 49 50 51 52 53 54 55 56 57 58 68 75 76 77 78 79 80 81 88 89
 102 103 104 106

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 40 41 42 43 44 45 59 60 61 62 63 64
 65 66 67 69 70 71 72 73 74 82 83 84 85 86 87

chain bonds :

4-22 6-106 7-11 8-24 11-15 12-16 12-20 13-17 13-21 14-18 14-19 19-23 25-26 26-27
 27-28 28-29 30-31 31-32 33-34 34-35 34-36 34-37 34-38 39-40 46-47 47-48 48-49
 50-51 51-52 52-53 54-55 56-57 58-59 68-69 75-76 76-77 77-78 78-79 79-80 80-81
 84-88 86-89 102-103 102-104

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9 10-11 10-14 11-12 12-13 13-14 40-41
 40-45 41-42 42-43 43-44 44-45 59-60 59-64 60-61 61-62 62-63 62-65 63-64 63-67
 65-66 66-67 69-70 69-74 70-71 71-72 72-73 73-74 82-83 82-87 83-84 84-85 85-86
 86-87

exact/norm bonds :

2-7 3-9 4-22 6-106 7-8 7-11 8-9 10-11 10-14 11-12 12-13 12-20 13-14 13-21 25-26
 39-40 46-47 48-49 50-51 54-55 58-59 62-65 63-67 65-66 66-67 68-69 102-103 102-104

exact bonds :

8-24 11-15 12-16 13-17 14-18 14-19 19-23 26-27 27-28 28-29 30-31 31-32 33-34 34-35
 34-36 34-37 34-38 47-48 51-52 52-53 56-57 75-76 76-77 77-78 78-79 79-80 80-81
 84-88 86-89

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45 59-60 59-64 60-61
 61-62 62-63 63-64 69-70 69-74 70-71 71-72 72-73 73-74 82-83 82-87 83-84 84-85
 85-86 86-87

G1:CN, [*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
 22:CLASS

23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:Atom 33:CLASS 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:Atom
41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS
51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:Atom 57:CLASS 58:CLASS 59:Atom 60:Atom
61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:CLASS 69:Atom 70:Atom
71:Atom 72:Atom 73:Atom 74:Atom 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
81:CLASS 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:CLASS 89:CLASS 102:CLASS
103:CLASS 104:CLASS 106:CLASS